The Role of Phonon Mechanism in Electron Coupling

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Abstract

In this article in the framework of generalized Frolich model we consider electron-spin-phonon system. A parameter of electron-spin-phonon interaction is found. It is shown its interrelation with experiments on isotope-effect on high temperature superconductors and asymptotic transformation to BCS theory [1, 2].

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Experimental study of high temperature superconductors have shown that electron-phonon interaction decreases with the raise of critical temperature T_c [3]. Thus electron coupling based only on phonon mechanism – the technique used to explain low temperature superconductivity – fails to explain high critical temperatures [4]. One can propose that in order to explain high T_c a theory with more complex mechanism in which the role of phonons decreases but does not vanish should be considered.

In this article in the framework of generalized Frolich model we will consider electron-spin-phonon interaction which is formed by the sum of electron-phonon, electron-spin and electron-spin-phonon interacting terms.

We start from the Hamiltonian of electron-spin-phonon system [5]

$$\hat{H}_{e+ph+s} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_s + \hat{H}_{e-ph} + \hat{H}_{e-s} + \hat{H}_{s-ph} + \hat{H}_{e-s-ph} \tag{1}$$

Now let us write the terms corresponding to the interaction of electrons with phonons and longitudinal spin modes

$$\hat{H}_{e-ph} = \frac{1}{\sqrt{V}} \sum \frac{g_{ph}}{\omega_D} i \sqrt{\frac{\hbar\omega_{ck\nu}}{2}} (n_\nu e_\nu)(\hat{b}_{k_1\nu} + \hat{b}^+_{-k_1\nu})\hat{c}^+_{k_2}\hat{c}_{(k_2-k_1)} \tag{2}$$

$$\hat{H}_{e-s} = \eta \frac{(p_{\nu e} n_\nu)}{\sqrt{\mu_e}} \frac{1}{\sqrt{V}} \sum i \sqrt{\frac{\hbar\omega_{sk}}{2}} (\hat{a}_{k_1 z} - \hat{a}^+_{-k_1 z})\hat{c}^+_{k_2}\hat{c}_{(k_2-k_1)} \tag{3}$$

$$\hat{H}_{e-s-ph} = \zeta\eta \frac{(p_{\nu' e} n_{\nu'})}{\sqrt{\mu_e}} (n_\nu e_3) \frac{1}{\sqrt{V}} \sum i \sqrt{\frac{\hbar\omega_{ck3}}{2}} (\hat{b}_{k_1 3} - \hat{b}^+_{-k_1 3})\hat{c}^+_{k_2}\hat{c}_{(k_2-k_1)} \tag{4}$$

here g_{ph}, ζ, η – are the coupling constants of electron and phonon subsystem, spin and phonon subsystem, electron and spin subsystem, a^+, a; b^+, b; c^+, c – creation and annihilation operators of magnons, phonons, and electrons, ω_D – is the Debye frequency, that is the maximum frequency of phonons which take part in the interaction, vectors e_ν represent phonon polarizations ($\nu = 1, 2, 3$), $n_\nu = k_\nu/|k_\nu|$, where k_ν is the wave vector, c – the sound velocity, $\omega_{sk} = J_0 s\sqrt{(k/k_c)^2 - 1}$ – the frequency of the longitudinal spin mode linearly coupled with phonons, J_0 – the exchange potential, $s = 1/2$ is the spin of electron, $k_c = 2\pi/r_c$, r_c – the exchange correlation radius, $\omega_{ck1,2} = ck$ and $\omega_{ck3} = ck\sqrt{1+\zeta^2}$ – the frequency of the phonon mode linearly coupled with the longitudinal spin mode, $p_{e\nu}$ – momentum of electron, μ_e – electron mass.

Using generalized Bogoliubov's transformation we represent operators a^+, a and b^+, b in the following form [6]

$$\hat{a}_{zk} = u_{zzk}\hat{c}_{zk} + v^*_{zz;-k}\hat{c}^+_{z;-k} + u_{z3k}\hat{d}_{3k} + v^*_{z3;-k}\hat{d}^+_{3;-k} \tag{5}$$

$$\hat{a}^+_{z;-k} = u^*_{zz;-k}\hat{c}^+_{z;-k} + v_{zzk}\hat{c}_{zk} + u^*_{z3;-k}\hat{d}^+_{-k;3} + v_{z3k}\hat{d}_{k;3} \tag{6}$$

$$\hat{b}_{3k} = u_{33k}\hat{d}_{3k} + v^*_{33;-k}\hat{d}^+_{3;-k} + u_{3zk}\hat{c}_{zk} + v^*_{3z;-k}\hat{c}^+_{z;-k} \tag{7}$$

$$\hat{b}^+_{3;-k} = u^*_{33;-k}\hat{d}^+_{3;-k} + v_{33k}\hat{d}_{3k} + u^*_{3z;-k}\hat{c}^+_{z;-k} + v_{3zk}\hat{c}_{3k} \tag{8}$$

The integral equation for the energy gap is given by

$$\Delta(\varepsilon) = \int_0^{\hbar\omega_c} \frac{\Delta(\varepsilon')}{\varepsilon'} Q(\varepsilon, \varepsilon') th \frac{\varepsilon'}{2T} d\varepsilon',$$

where ω_c is close to the order of maximum coupled spin-phonon oscillations. The kernel of this integral equation can be written in the form $Q = Q_{e-ph} + Q_{e-s} + Q_{e-s-ph}$. Each term can be presented as the sum of the Green functions using coefficients in (2)-(4) [7]. Considering the long-waves limit we get

$$Q_{e-ph}(k) = N(0)\frac{2g_{ph}^2}{3\omega_{D_0}} + N(0)\frac{g_{ph}^2}{3\omega_{D_0}\sqrt{1+\zeta^2}}[|u_{33k}+v_{33k}|^2\frac{\omega_{ck3}}{\varepsilon_{3k}} + |u_{3zk}+v_{3zk}|^2\frac{\omega_{ck3}}{\varepsilon_{sk}}]$$

$$Q_{e-s}(k) = N(0)\frac{p_F^2}{3\mu_e}\eta^2[|u_{zzk} - v_{zzk}|^2\frac{\omega_{sk}}{\varepsilon_{sk}} + |u_{z3k} - v_{z3k}|^2\frac{\omega_{sk}}{\varepsilon_{3k}}] \tag{9}$$

$$Q_{e-s-ph}(k) = N(0)\zeta^2\frac{p_F^2}{9\mu_e}\eta^2[|u_{33k} - v_{33k}|^2\frac{\omega_{ck3}}{\varepsilon_{3k}} + |u_{3zk} - v_{3zk}|^2\frac{\omega_{ck3}}{\varepsilon_{sk}}]$$

here ω_{D_0} – is the representative value of Debye frequency in the BCS theory of low temperature superconductors, while $\omega_{D_1} = \omega_{D_0}\sqrt{1+\zeta^2}$ is the Debye frequency in the electron-spin-phonon system, ε_{sk} and ε_{3k} – are the frequencies of coupled spin-phonon oscillations, and $N(0)$ – is the density of electron states on Fermi surface. Please note that g_{ph} is equal to zero when $k > 2k_F$, while ζ and η are constants.

Let us now consider the additional contribution to the Coulomb repulsion of electrons which appears as a result of spin-electron interaction. In the simplest case of isotropic Fermi surface this contribution is given by [8]

$$\Delta\mu = N(0)\frac{p_F^2}{3\mu_e}\eta^2 \tag{10}$$

Now let us write the value of $Q_{e-s}(k)$ with this contribution

$$Q_{e-s}(k) = N(0)\frac{p_F^2}{3\mu_e}\eta^2[|u_{zzk} - v_{zzk}|^2\frac{\omega_{sk}}{\varepsilon_{sk}} + |u_{z3k} - v_{z3k}|^2\frac{\omega_{sk}}{\varepsilon_{3k}} - 1] \tag{11}$$

Substituting the explicit values of functions u_{33k}, v_{33k}, u_{3zk}, v_{3zk}, u_{z3k}, v_{z3k}, u_{zzk}, v_{zzk}, to (9), (11) we obtain

$$Q_{e-ph}(k) = N(0)\frac{2g_{ph}^2}{3\omega_{D_0}} + \nu(\varepsilon_F)\frac{g_{ph}^2}{3\omega_{D_0}\sqrt{1+\zeta^2}}q_{e-ph}(k)$$

$$Q_{e-s}(k) = N(0)\frac{p_F^2}{3\mu_e}\eta^2\left[q_{e-s} - 1\right] \tag{12}$$

$$Q_{e-s-ph}(k) = N(0)\frac{p_F^2}{9\mu_e}\eta^2\zeta^2 q_{e-s-ph}(k)$$

where

$$q_{e-ph}(k) = \frac{z^2\omega_{sk}^2\omega_{ck3}^2}{(\varepsilon_{3k}^2 - \varepsilon_{sk}^2)(\varepsilon_{3k}^2 - \omega_{ck3}^2)} + \frac{(\varepsilon_{sk}^2 - \omega_{sk}^2)}{(\varepsilon_{sk}^2 - \varepsilon_{3k}^2)}$$

$$q_{e-s}(k) = \frac{z^2\omega_{sk}^4\omega_{ck3}^2}{\varepsilon_{sk}^2(\varepsilon_{sk}^2 - \varepsilon_{3k}^2)(\varepsilon_{sk}^2 - \omega_{sk}^2)} + \frac{\omega_{sk}^2(\varepsilon_{3k}^2 - \omega_{ck3}^2)}{\varepsilon_{3k}^2(\varepsilon_{3k}^2 - \varepsilon_{sk}^2)}$$

$$q_{e-s-ph}(k) = \frac{z^2\omega_{sk}^2\omega_{ck3}^4}{\varepsilon_{3k}^2(\varepsilon_{3k}^2 - \varepsilon_{sk}^2)(\varepsilon_{3k}^2 - \omega_{3k}^2)} + \frac{\omega_{3k}^2(\varepsilon_{sk}^2 - \omega_{sk}^2)}{\varepsilon_{sk}^2(\varepsilon_{sk}^2 - \varepsilon_{3k}^2)}$$

Let us now compute $Q_{e-ph}(k)$, $Q_{e-s}(k)$, and $Q_{e-s-ph}(k)$ explicitly. We introduce the following functions

$$w_{e-ph} = q_{e-ph}(k); \tag{13}$$

$$w_{e-s} = \frac{1}{1+\zeta^2}q_{e-s}(k);$$

$$w_{e-s-ph} = \frac{1}{1+\zeta^2}q_{e-s-ph}(k).$$

For $k > k_c$ the functions w_{e-ph}, w_{e-s}, and w_{e-s-ph} are equal to 1. Let us note that since the pairing is performed in the range $r < r_c$ and $k_c = 2\pi/r_c$ the range $k > k_c$ is of our interest. Thus using (13) we get

$$q_{e-ph}(k) = 1; \tag{14}$$

$$q_{e-s}(k) = 1 + \zeta^2;$$

$$q_{e-s-ph}(k) = 1 + \zeta^2.$$

Results of numerical simulation of these functions are presented on Fig.1.

Using these results we simplify (12) getting

$$Q_{e-ph}(k) = N(0)\frac{2g_{ph}^2}{3\omega_{D_0}} + N(0)\frac{g_{ph}^2}{3\omega_{D_0}\sqrt{1+\zeta^2}} \tag{15}$$

$$Q_{e-s}(k) = N(0)\frac{p_F^2}{3\mu_e}\eta^2\zeta^2$$

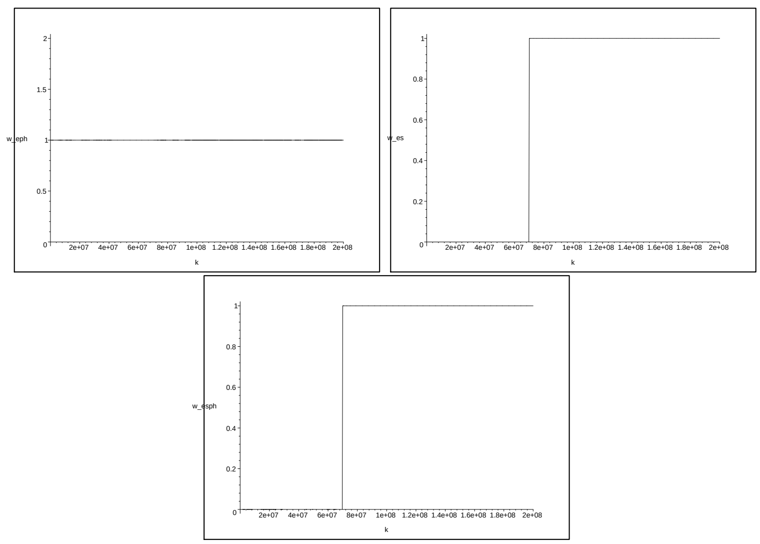

Figure 1: The results of numerical simulation of the functions w_{e-ph}, w_{e-s} and w_{e-s-ph} (13). These plots illustrates the equalities (14). The upper left is the plot of w_{e-ph} as a function of k, the upper right shows the picture of w_{e-s}, and the lower – w_{e-s-ph}. Let us note that for the values of ζ in the range $0 < \zeta < 10$ all functions (13) have the same form. One can see that for $k > k_c$, i.e. in the area where the coupling is performed the functions w_{e-ph}, w_{e-s}, and w_{e-s-ph} are equal to 1.

$$Q_{e-s-ph}(k) = N(0)\zeta^2 \frac{p_F^2}{9\mu_e}\eta^2(1+\zeta^2).$$

Now $Q(k)$ will be

$$Q(k) = N(0)\left[\frac{2g_{ph}^2}{3\omega_{D_0}} + \frac{g_{ph}^2}{3\omega_{D_0}\sqrt{1+\zeta^2}} + \frac{p_F^2}{9\mu_e}\zeta^2\eta^2(4+\zeta^2)\right] \tag{16}$$

Let us consider two frequency ranges. The range $\omega < \omega_{D_0}$ corresponds to low temperature super conductivity, while the range $\omega > \omega_{D_0}$ corresponds to high temperature superconductivity.

In the range $\omega > \omega_{D_0}$ the expression (16) takes the form

$$Q(k) = N(0)\left[\frac{g_{ph}^2}{3\omega_{D_0}\sqrt{1+\zeta^2}} + \frac{p_F^2}{9\mu_e}\zeta^2\eta^2(4+\zeta^2)\right] \tag{17}$$

From (17) we see that electron-phonon interaction decreases with the raise of critical temperature (that is with the raise of frequency). This fact is supported by experiments on isotope-effect, which shows that electron-phonon interaction should be taken into consideration [9]. Although since electron-phonon interaction alone is not enough to explain high critical temperatures, one should consider more complex interaction, like spin-electron-phonon interaction, as it is done in the present work.It was shown in experiments on La_2CuO_4 that for $T > T_N$ spin fluctuations have high energy and the velocity of spin fluctuations ($\sim 10^6$ cm/s) is greater than the sound velocity ($\sim 10^5$ cm/s) [10].

In the range $\omega < \omega_{D_0}$ we have

$$\zeta = \frac{\sqrt{3}g\hbar k_c}{\sqrt{J_0 s M}} \to 0$$

here M is the reduced mass of ion, $g = U/J_0$, where U is the electron-ion potential. Now the expression (16) takes the form

$$Q(k) = N(0)\frac{g_{ph}^2}{\omega_{D_0}},$$

which is exactly the electron-phonon interaction term in BCS theory.

Let us note that spin fluctuations exist in all superconductors. Although in low temperature superconductors this fluctuations are small and thus do

not seriously affect electron coupling[11, 12, 13]. On the other hand in high temperature superconductors these fluctuations increases due to the second term in (17).

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